

# DL-Valine, N-methyl-N-hexyloxycarbonyl-, butyl ester

<b>Inchi:</b>	InChI=1S/C17H33NO4/c1-6-8-10-11-13-22-17(20)18(5)15(14(3)4)16(19)21-12-9-7-2/h14
<b>InchiKey:</b>	ZYHNTLOFHOUXSL-UHFFFAOYSA-N
<b>Formula:</b>	C17H33NO4
<b>SMILES:</b>	CCCCCOC(=O)N(C)C(C(=O)OCCCC)C(C)C
<b>Mol. weight [g/mol]:</b>	315.45

## Physical Properties

Property code	Value	Unit	Source
gf	-269.68	kJ/mol	Joback Method
hf	-826.84	kJ/mol	Joback Method
hfus	41.33	kJ/mol	Joback Method
hvap	73.02	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.003		Crippen Method
mvol	275.250	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	1963.00		NIST Webbook
rinpol	1963.00		NIST Webbook
tb	752.50	K	Joback Method
tc	933.04	K	Joback Method
tf	428.14	K	Joback Method
vc	1.042	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.02	J/mol×K	752.50	Joback Method
cpg	851.50	J/mol×K	782.59	Joback Method
cpg	868.03	J/mol×K	812.68	Joback Method
cpg	883.63	J/mol×K	842.77	Joback Method
cpg	898.30	J/mol×K	872.86	Joback Method
cpg	912.07	J/mol×K	902.95	Joback Method
cpg	924.95	J/mol×K	933.04	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392887&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392887&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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